Electronic Supplementary Material for

Visualising the equilibrium distribution and mobility of organic contaminants in soil using the chemical partitioning space

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SI-1 Phase parameters and solute descriptors

Phase parameters for the pp-LFERs used in the construction of phase partitioning space maps.

Phase parameters	s	a	b	l	v	c	Ref
Pahokee peat/water (25 °C)	-0.98	-0.42	-3.34	0.54	1.20	0.02	1
Leonardite humic acid/water (40 °C)	-1.15	-0.64	-2.95	0.21	2.45	0.57	2
Leonardite humic acid/water (25 °C)	-0.93	-0.43	-3.14	0.25	2.49	0.26	2
Leonardite humic acid/water (15 °C)	-0.79	-0.29	-3.26	0.28	2.51	0.05	2
Leonardite humic acid/water (5 °C)	-0.65	-0.15	-3.39	0.31	2.53	-0.15	2
Air/water (40 °C)	-1.95	-3.43	-4.62	-0.51	2.86	0.60	3
Air/water (25 °C)	-1.94	-3.68	-4.97	-0.52	2.68	0.51	3
Air/water (15 °C)	-1.93	-3.85	-5.20	-0.52	2.56	0.45	3
Air/water (5 °C)	-1.92	-4.02	-5.43	-0.52	2.44	0.39	3

Note: The phase parameters were calculated at different temperatures using linear correlations between phase descriptors and temperature reported in ref 2 for Leonardite humic acid/water, and ref 3 for air/water. The phase parameters for Pahokee peat/water were taken from eq. 6 of ref. 1.

References

1. G. Bronner and K.-U. Goss, *Environ. Sci. Technol.*, 2011, **45**. 1313-1319.
2. C. Niederer, K. U. Goss and R. P. Schwarzenbach, *Environ. Sci. Technol.*, 2006, **40**, 5374-5379.
3. K. U. Goss, *Chemosphere*, 2006, **64**, 1369-1374.

Solute descriptors

Chemical	S	A	B	L	V	Ref [S, A, B, V]	Ref [L]
Amitrole	0.86	1.11	0.35	2.61	0.60	1	2
Atrazine	1.28	-0.01	0.96	7.34	1.62	3	3
Bromacil	1.08	0.87	0.83	8.18	1.63	3	3
Chlorothalonil	2.20	-0.25	0.44	7.65	1.52	3	3
Chlorpyrifos	0.34	0.00	1.11	8.57	2.15	1	2
Cypermethrin	0.24	0.02	1.55	11.87	2.97	1	2
Cyromazine	0.03	1.36	1.17	4.92	1.207	1	2
Desethylatrazine	1.07	0.37	0.88	6.67	1.34	3	3
Endosulfan	0.82	0.41	0.96	9.38	2.08	3	3
Endrin	1.28	0.00	0.38	8.06	2.01	1	2
Metolachlor	0.95	0.09	1.35	8.86	2.28	3	3
Carbamazepine	2.00	0.42	0.90	9.40	1.81	3	3
Fluorouracil	0.67	1.05	0.77	3.81	0.77	1	2
Triclosan	1.81	0.92	0.3	8.96	1.81	3	3
Zearalenone	1.68	0.87	1.24	11.95	2.46	3	3
1,1,1-trichloroethane (TCE)	0.41	0	0.09	2.73	0.76	4	4
p-xylene	0.52	0	0.16	3.84	1.00	5	4
PCB-52	1.33	0	0	8.49	1.64	6	2
PCB-101	1.47	0	0	9.22	1.76	6	2
PCB-138	1.61	0	0	9.95	1.88	6	2

Note: If an experimental *L* was not available, *L* was determined according to eq. SI19 in ref. 2.

Refereneces

1. H. C. Tülp, K. U. Goss, R. P. Schwarzenbach and K. Fenner, *Environ. Sci. Technol.*, 2008, **42**, 2034-2040.
2. T. N. Brown, and F. Wania, *Environ. Sci. Technol.*, 2009, **43**, 6676-6683.
3. G. Bronner, and K.-U. Goss, *Environ. Sci. Technol.*, 2010, in press.
4. M. H. Abraham, J. Andonianhaftvan, G. S. Whiting, A. Leo and R. S. Taft, *J. Chem. Soc.-Perkin Transact. 2*, 1994, 1777-1791.
5. M. H. Abraham, and M. Roses, *J. Phy. Organic Chemical.*, 1994, **7**, 672-684.
6. P. C. M. van Noort, J. J. H. Haftka and J. R. Parsons, *Environ. Sci. Technol.*, 2010, **44**, 7037-7042.

SI-2 Expressing the humidity and temperature dependence of surface adsorption.

Goss et al.[1] reported experimental K_{IA} for a range of chemicals at different relative humidity at 15°C. Using these data, humidity dependent phase descriptors for K_{IA} were derived for RH>90% and <90%. These are summarized in Table S1.

Table S1 Slopes and intercepts of the humidity dependent phase descriptors.

Phase Descriptor	Slope (S) Intercept (I)	K_{IA} (RH<=90%)	K_{IA} (RH>90%)
A	Sa_{ju}	-0.00125	0.01
	Ia_{ju}	1.0142	1.11E-16
B	Sb_{ju}	-0.0025	0.01
	Ib_{ju}	1.125	1.11E-16
L	Sl_{ju}	-0.035	0
	Il_{ju}	7.7167	4.6

K_{IA} is subsequently adjusted to different temperatures according to eq [S1]. No pp-LFER equation could be obtained for ΔU_{IA}. To implement temperature dependence for K_{IA} an empirical equation derived by Goss and Schwarzenbach[2] was modified to calculate the inner energy of phase transfer from the K_{IA} as shown in eq [S2]. A factor of 1000 has been included to yield an adsorption enthalpy in J/mol, and an additional term was added to convert the result from an enthalpy to an inner energy as discussed by Goss[3].

$$K_{IA}^{T2} = K_{IA}^{T1} \cdot \exp[-\frac{\Delta U_{IA}}{R}(\frac{1}{T_2} - \frac{1}{T_1})] \qquad \text{Eq [S1]}$$

$$\Delta U_{IA}(J/mol) = (-4.57 \cdot \ln K_{IA}^{T1} - 92.2) \cdot 1000 + R \cdot 298.15 \qquad \text{Eq [S2]}$$

References

1. K. U. Goss, J. Buschmann and R. P. Schwarzenbach, *Environ. Sci. Technol.*, 2004, **38**, 3667-3673.
2. K. U. Goss, and R. P. Schwarzenbach, *Environ. Sci. Technol.*, 1999, **33**, 3390-3393.
3. K. U. Goss, *Chemosphere*, 2006, **64**, 1369-1374.